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Project Summary

A Model of Turbulent Diffusion Flames and Nitric Oxide Generation

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A new view is described of mixing and chemical reactions in turbulent fuel jets discharging into air. Review of available fundamental data from jet flames leads to the idea that mixing begins with a large scale, inviscid, intertwining of entrained air and fuel throughout the jet. Significant molecular mixing is delayed until the end of a cascade to the Kolmogorov scale. A simple mathematical model incorporating these ideas is presented. This model predicts a Reynolds number dependence for the nitric oxide (NO) formation rate that is in good agreement with measurements in both methane (CH_4) and hydrogen (H_2) jets burning in air. These mathematical model concepts have been incorporated into a simplified computer program capable of treating the detailed chemical kinetics of a gas flame. The model has been used to predict NO formation in H_2/air and CH_4/air flames. Results compare favorably with experimental data.

This Project Summary was developed by EPA's Air and Energy Engineering Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

A central focus of EPA's combustion research program has been development of combustion control technologies to limit formation of nitrogen oxides (NO_x) from fossil fuel fired flames. The Fundamental Combustion Research (FCR) program has helped advance understanding of critical combustion processes controlling NO_x formation. As part of the FCR program a series of studies have been pursued to develop an improved understanding of the coupling between fundamental fluid mechanics and chemical processes in turbulent diffusion flames. The impetus for these efforts is twofold: (1) control of mixing between fuel and combustion air is a central feature in low NO_x burner systems (by delaying the mixing, more of the fuel nitrogen in coal reacts under fuel rich conditions which is conducive to converting the bound nitrogen to molecular nitrogen); and (2) the more fundamental impetus is that since the middle 1970s a new understanding of basic turbulent mixing processes has been evolving. The current FCR study provided for development of a mathematical model of a simple turbulent diffusion jet flame incorporating the basic elements from the new understanding of turbulent mixing. The flow configuration modeled in this study is a circular jet of gaseous fuel issuing into still air.

The Basic Concept

The new understanding of turbulence is based on the concept that mixing between fuel and air is initially driven by large coherent structures (often referred to as eddies) which macroscopically entrain air and engulf it into the fuel jet. Both theoretical considerations and experimental data show that the macroscopic entrainment of a turbulent jet (at high Reynolds number) becomes independent of Reynolds number and is

linearly proportional to the axial distance. The large structures transport engulfed material deep within the jet with mixing between fuel and air occuring at the interface between the fluids. At any axial location macroscopically entrained fluid is molecularly mixed at a uniform rate with the jet fluid. This leads to the concept, supported by experimental data, that there is no radial variation of the reservoir-jet mixture ratio *in the mixed fluid*. In this view, the usual bell-shaped *mean* concentration profiles arise only from a radial variation in the ratio of mixed fluid to pure reservoir fluid.

Additional features of the model are that mixing takes place at the interface surfaces (or flame sheet) separating fuel and oxidizer and that the combustion is at stoichiometric conditions. The interface surface associated with the large scale structures break down to small scale through inviscid instable motion. This cascade of length scales causes the quantity of interface surface area to increase: most of the surface being generated just before the structures reach the Kolmogorov scale. The interface surfaces are homogenized by molecular diffusion at this scale.

Process is Modelled

This rather complex process has been modelled as a combination of two major combustion zones: a flame sheet zone and a flame core zone. The flame sheet zone represents the interface between fuel and air where combustion is occurring at stoichiometric conditions. The characteristic scale for this zone is the Kolmogorov scale since that is the scale where most of the interface surface is generated. The flame core zone consists of the mixture of the combustion products and the as-yet unreacted fuel which are molecularly mixed. After its formation, the flame sheet zone subsequently conglomerates into the flame core structure via molecular diffusion. Numerically, the flame sheet zone can be simulated by a well stirred reactor with proper characteristic residence time. The flame core zone can be represented by a plug flow reactor, which originally contains 100% raw fuel, and is continuously fed by the combustion products from the flame sheet reactor. In the meantime, the flame core zone also has to provide the flame sheet reactor with the rich mixture which contains a sufficient amount of raw fuel for stoichiometric combustion (corresponding to the rate of microscopic mixing of fresh air). The above ideas are best described with the help of Figure 1 which presents a schematic of the reactor arrangement. The term

$$\frac{d}{dt}\left(\frac{m_a}{m_o}\right)_{micro}$$

represents air engulfed into the jet by large scale structure which subsequently cascades to the Kolmogorov scale. This air addition rate is matched stoichiometrically by fuel addition from the flame core

$$\left[\frac{d}{dt}\left(\frac{m_{fc}}{m_o}\right)_{micro}\right]$$

These two streams react in the well stirred reactor representing the flame sheet zone. Combustion products from the flame sheet zone flow to the flame core zone, diluting the fuel in the plug flow reactor.

The numerical model embodying the above concepts provided a simple treatment for heat loss by radiation and used an existing one-dimensional chemical reactor code. The governing species and energy equations for both reactors are solved using a fully implicit, backward finite difference formulation. Reaction chemistry was described using a set of 181 simultaneous elementary reactions and 36 species for CH_4/air flames. This reaction set was developed previously as part of the FCR program and includes treatment of thermal NO and fuel nitrogen mechanisms. For H_2/air flames the kinetic set can be reduced to 17 species and 60 elementary reactions.

After developing the model and empirically establishing values for necessary constants the computer code was exercised to predict flame characteristics which could be compared to experimental data. Figure 2 illustrates one of those comparisons in a plot of the NO mass fraction at the jet center line versus the axial distance down the flame. Model predictions are compared to the experimental data of Bilger and Beck [presented at 15th Symposium (International) on Combustion]. The flames simulated in this figure used hydrogen as the fuel and the general agreement of prediction and theory is encouraging.

Additional work is required to fully test the model under critical conditions and to better establish the empirically set constants. Analysis of model predictions may provide valuable insights into basic

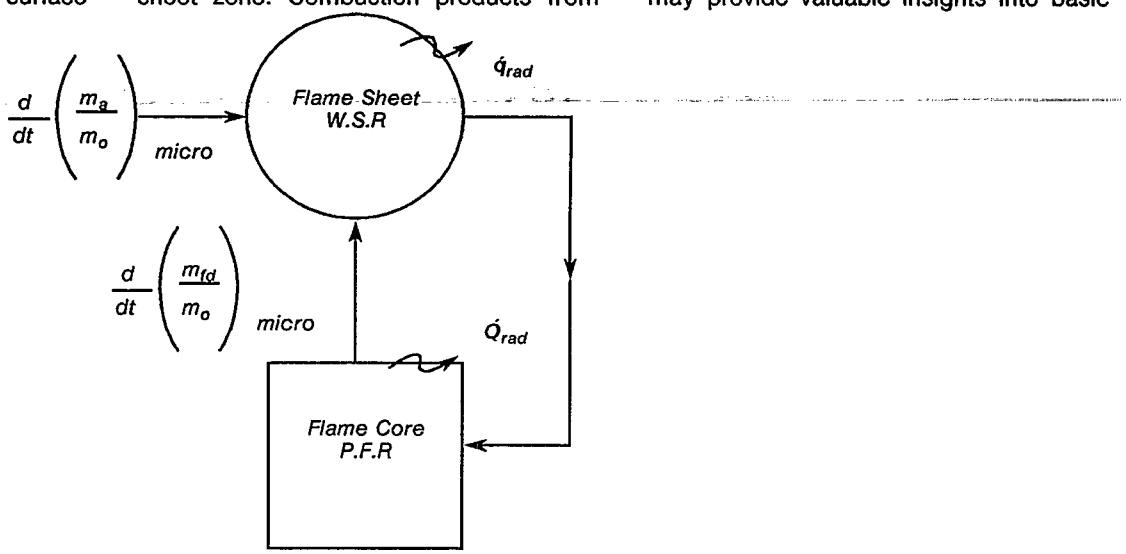

Figure 1. Schematic of reactor model.

processes controlling NO emissions. Limited analysis shows that NO_x formation occurs in the flame sheet zone, while the flame core zone provides strong NO destruction. This NO_x result is as expected, but the ability to evaluate the separate roles of different regions of the flame could be of significant value in future NO_x control studies.

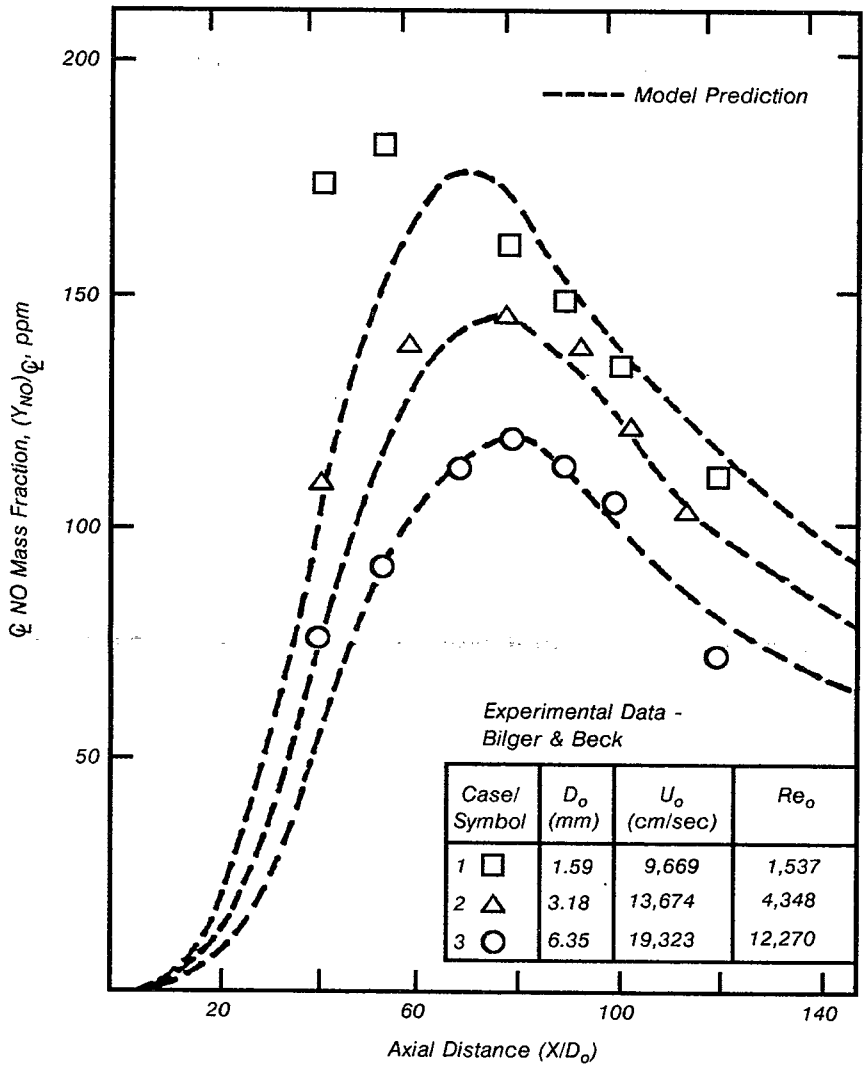

Figure 2. Comparison of model calculated NO versus measurements ($Fr = 6 \times 10^{-5}$) for H_2/air flames.

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The complete report, entitled "A Model of Turbulent Diffusion Flames and Nitric Oxide Generation," (Order No. PB 90-155 557/AS; Cost: $17.00, subject to change) will be available only from:
National Technical Information Service
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